VARIATIONAL PRINCIPLE AND THE HARMONIC OSCILLATOR

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.1.

We've covered the variational principle before while studying Griffiths's book, but Shankar provides a few new examples which are worth going through. In this example, we look at the harmonic oscillator and use the trial function

$$\psi = Ae^{-\alpha x^2} \tag{1}$$

where A is the normalization constant and α is the parameter to be varied in an attempt to get the best estimate for the ground state energy. [Of course, we already know that the exact ground state wave function has this form, so this exercise can be viewed more as a demonstration that the variational principle can give the exact answer if the right form of trial function is used.]

First we find A from the condition

$$\int_{-\infty}^{\infty} \psi^2 dx = A^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = 1 \tag{2}$$

This is a standard Gaussian integral, but I've used Maple to do the integrals here. We have

$$\int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = \sqrt{\frac{\pi}{2\alpha}} \tag{3}$$

so

$$A = \left(\frac{2\alpha}{\pi}\right)^{1/4} \tag{4}$$

We can now apply the variational principle. We must find

$$\langle \psi | H | \psi \rangle = \sqrt{\frac{2\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha x^2} \left(-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 e^{-\alpha x^2} \right) dx \tag{5}$$

The first term in the integrand is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=-\frac{\hbar^2\alpha}{m}\left(2\alpha x^2-1\right)e^{-\alpha x^2} \tag{6}$$

Thus

(7)

$$\langle E\rangle=\langle\psi|H|\psi\rangle=\sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}e^{-2\alpha x^2}\left[-\frac{\hbar^2\alpha}{m}\left(2\alpha x^2-1\right)+\frac{1}{2}m\omega^2x^2\right]dx$$

$$=\sqrt{\frac{2\alpha}{\pi}}\left[\left(\frac{1}{2}m\omega^2-\frac{2\hbar^2\alpha^2}{m}\right)\int_{-\infty}^{\infty}x^2e^{-2\alpha x^2}dx+\right. \tag{8}$$

$$\left.\frac{\hbar^2\alpha}{m}\int_{-\infty}^{\infty}e^{-2\alpha x^2}dx\right] \tag{9}$$

$$=\frac{\hbar^2\alpha}{2m}+\frac{m\omega^2}{8\alpha} \tag{10}$$

where I used Maple to do the integrals and simplify the result to get the last line. If you want to do them by hand, the two integrals are standard Gaussian integrals so you should be able to do them by looking them up in tables.

We now find the optimum value of α by differentiating:

$$\frac{d\langle E\rangle}{d\alpha}=\frac{\hbar^2}{2m}-\frac{m\omega^2}{8\alpha^2}=0 \tag{11}$$

Solving, we find

$$\alpha_0=\frac{m\omega}{2\hbar} \tag{12}$$

(There is also a negative root, but we know $\alpha>0$ to prevent the wave function blowing up at infinity.)

Substituting into 10 we get the energy as

$$E_0=\frac{1}{2}\hbar\omega \tag{13}$$

which is the exact ground state energy.